NUMERICAL SIMULATION OF 2-D POLLUTANT TRANSPORT IN OPEN CHANNELS

A Thesis Submitted
in Partial Fulfilment of the Requirements
for the Degree of
MASTER OF TECHNOLOGY

by

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to the

Department of Civil Engineering
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October, 1996

CERTIFICATE

This is to certify that the the work contained in the thesis entitled Numerical Simulation of 2-D Pollutant Transport in Open Channels *has been carried out by* VEMPATI BHASKARA SRI RAMA LINGESWARA SARMA *under my supervision and it has not been submitted elsewhere for a degree.*

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ABSTRACT

A numerical simulation model for 1-D steady state flow in open channels with irregular non-uniform cross section and a numerical simulation model for 2-D pollutant transport using a modified form of the mixing analysis based on the concept of stream tubes(MABOCOST) are presented. Gradually varied flow(GVF) in the channel is considered.The flow simulation model is formulated using the fourth order Runge Kutta method. The flow model is solved for an open channel with specified irregular cross sections assuming immobile bed conditions.The transport simulation model utilizes the flow simulation solutions to simulate pollutant transport in the channel,assuming advective and dispersive transport processes.The transport model simulates the spatial and temporal distribution of pollutant concentration for given pollution sources.The simulated results are compared with reported experimental results for a similar 2-D system as well as reported 2-D simulation results using MABOCOST.These comparisions and mass balance analysis show that the combined 1-D flow and 2-D pollutant transport simulation results may be used as approximate solutions for the 2-D system for preliminary assessment.Both conservative pollutants and pollutants undergoing decay process are considered.

ACKNOWLEDGEMENTS

I express my profound sense of gratitude to my teacher **Dr. Bithin Datta** for suggesting the problem of this thesis and his guidance throughout the work. It was a memorable and enjoyable experience to work with him.

I am thankful to the staff of Civil Engineering Department especially my teachers Dr. B.S. Murty, Dr. T. Gangadhariah, Dr. K.Subramanya, Dr.S.Surya Rao and Dr. S.Ramaseshan who enforced my foundations in Civil Engineering.

I also thank my friends and all well wishers for their cooperation and encouragement in completing my mission.

Finally, I wish to express my gratitude to the Department of Science and Technology for the financial support.

- VEMPATI B S R L SARMA

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NOTATION

A	cross-sectional area of discharge (m^2)
C	depth-averaged concentration (mg/L)
D	dispersion factor (s^{-1})
E_x	longitudinal mixing coefficient (m^2/s)
E_z	transverse mixing coefficient (m^2/s)
g	accelaration due to gravity $(m/s^2))$
h	flow depth of stream channel (m)
L	ratio between distance travelled in time step to longitudinal length of grid element
l_n	fraction of overlapping area of element with its nth adjacent element on left
m_x, m_z	longitudinal and transverse metric coefficients respectively in stream-tube equation
n	Manning's coefficient of roughness
n	normalized cumulative discharge $(\frac{q}{Q})$
Q	flow rate of stream channel (m^3/s)
q	cumulative discharge (m^3/s)
R	hydraulic radius of the stream channel (m)
r_n	fraction of overlapping area of element with its nth adjacent element on right

S_0	bottom slope of the stream channel
S_f	energy slope of the channel flow
T	top width of flow cross-section (m)
t	time (s)
u	depth-averaged longitudinal velocity (m/s)
x	longitudinal coordinate axis (m)
y	depth of flow with respect to a datum (m)
z	transverse coordinate axis (m)
α	rate of growth or decay of pollutant (s^{-1})
β	magnitudeof source-sink term $(mg/L)(L/s)$
ΔC	concentration surplus between element and its neighbor, (mg/L)
Θ	stream-tube element volume m^3)

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Chapter 1

Introduction

1.1 Introduction

The human interference in the natural activities can be seen through so many environmental hazards. The manifestation of such an interference is poor water quality in natural Rivers which is ultimately causing great problems in maintaining ecological balance. As such it has long been noted that the problem of poor water quality in the natural rivers interferes with the human life and the manifestation of that interference is indicated by disease transmission and aesthetic nuisances. Nowadays, water quality in natural sreams is becoming a major issue all over the world due to wide spread pollution. Hence, the necessity of evolving effective remedial measures are being very important.

On the contrary, modelling the transport of pollutants is difficult due to nature's hetrogeneity and the complexity of estimating the flow and transport parameters especially, in natural flow systems like meanders, irregular cross sections, tributaries and lateral flows. Due to these complexities, an effective control of pollution and maintaining aesthetic conditions in natural streams requires development and solution of water quality models taking into consideration the complete processes involved.

In this study (i) A numerical model is developed for simulating 1-D flow under steady state conditions for channels with irregular cross sections (ii) A simulation

model is solved for simulating the 2-D transport of a pollutant in the channel. This model is applicable for both 1-D and 2-D flow systems using the stream tube concept.

The transport model simulates the spatial and temporal distribution of pollutant concentration for given pollution sources. The simulatoion results for 1-D simulation are compared with reported experimental results for a similar 2-D system as well as reported 2-D simulation results using MABOCOST. These comparisions and mass balance analysis show that the 1-D simulation results can be used as approximate solutions for the 2-D system for preliminary assessment. Both conservative pollutants and pollutants undergoing decay process are considered.

1.2 Literature Review

A steady non-uniform flow in a channel with gradual changes in its water surface elevation is termed as gradually-varied flow (GVF). In GVF, the depth of flow and velocity vary along the channel. The bed slope, water surface slope, and energy slope will all differ from each other. Because of its practical importance the computation of GVF has been a topic of continued interest for somany years.

To meet the practical needs, various solution procedures involving graphical and numerical methods were evolved. The advent of high speed computers has given rise to general programmes utilizing sophisticated numerical techniques for solving GVF in natural channels. The various available procedures for computing GVF profiles can be classified as:

1. Direct integration

2. Numerical method

3. Graphical method

Computation procedures applicable to an artificial channel may not be directly applicable to natural channels (Subramanya,1989) of irregular cross section since in a natural channel, the cross sectional properties are known only at specified locations while in prismatic artificial channel the cross-sections are generally constant all along

the channel. Because of this, some methods have been developed, particularly for use in natural channels, e.g. Standard-step metod.

The numerical solution procedures to solve GVF problems can be broadly classified into two categories as:

(I) Simple Numerical Methods

(II) Advanced Numerical Methods

Simple numerical methods usually attempt to solve the energy equation either in the form of the differential energy equation of GVF or in the form of the Bernouli equation. Two commonly used simple numerical methods to solve GVF problems are as follows:

(i) Direct-step method and

(ii) Standard step method

Advanced numerical methods are normally suitable for use in digital computers as they involve a large number of repeated calculations. The basic differential equation of GVF can be expressed as a function of depth of flow only for a given bed slope, Manning's coefficient of roughness, flow and channel geometry. A class of methods which is particularly suitable for numerical solution of this non-linear equation is the Runge-Kutta method. There are different orders of Runge-Kutta methods and all of them evaluate the depth of flow at a desired section provided the depth at a known section is given. The fourth order method is used here for its accuracy. The various numerical methods are as follows:

(a) Standard Fourth Order Runge-Kutta Method (SRK)

(b) Kutta-Merson Method (KM)

(c) Trapezoidal Method (TRAP)

Studies have been reported (in Subramanya,1989) by Apelt (1971) and Humpridge and Moss (1972) on the SRK method;by Apelt on the KM and TRAP methods and

by Prasad (1970) on the TRAP method. It has been found that all these three methods are capable of direct determination of the GVF profiles both in upstream and down stream directions irrespective of the nature of flow, i.e whether the flow is subcritical or super critical. It has been observed that the SRK and KM methods require less computational effort than TRAP method. Also, while the SRK method is slightly more efficient than the KM method, the possibility of providing automatic control of the step size and accuracy in the KM process makes it a strong contender. Though there are host of Graphical methods, these have become obsolete with the advent of easy access to digital computers. In this study SRK method is adopted for computation.

The Preissmann scheme (Chaudhary,1990) has been extensively used for the past three decades. It has the advantages that a variable spatial grid may be used. By varying the weighting coefficient steep wave fronts may be properly simulated. Preissmann scheme yields an exact solution of the linearized form of the governing equation for a particular value of step size in both the directions of length and time.

For N number of reaches on the channel this scheme yields $2N$ equations for each grid point. The equations cannot be written for the grid points at the downstream end. However, the number of unknowns are $2(N+1)$, that is, two unknowns for each grid point. Thus, two more equations are needed for a unique solution. These are provided by the end conditions. Unlike the explicit schemes, the equations describing the end conditions are directly included in the system of equations. In other words, we do not have to use the characteristic equations or the reflection procedures. Because steady state conditions are assumed in this solution, the SRK method is adopted.

The scheme is unconditionally stable provided the flow variables are weighted towards the next higher time level. An unconditional stability means that there is no restriction on the step size of both the length and time. However, for accuracy the courant number should be close to 1.0 for frictionless channel. But if linearized form of the friction loss term is included in the analysis then Vedernikov number should be close to 1.0

As far as pollution transport in streams is concerned, mathematical models of different levels of sophistication, based on some finite difference representations of mass balance equation, have been developed. The mixing model is based either on the rectangular channel assumption or the stream tube concept (Beltaos,1979; Paily and Sayre,1978; Rood and Holley,1974; Stefan and Gulliver,1978; Yotsukura,1977; Yotsukura and Cobb,1972). The latter class of models have become more popular in recent years because of their ability to simulate processes in natural stream channels having irregular cross sections. Numerical models are far more advantageous than analytical models, with respect to flexibility, as they provide the capability of accounting for actual flow patterns and boundary geometry as well as spatially varying mixing parameters.

Most of the mixing models developed to-date are one-dimensional in nature, that is, complete mixing of pollutants across the stream sections is assumed. Models given by Fukuoka and Sayre (1973), Valentine and Wood (1977), Beltaos(1980), Terragni and Young (1983) and McBribe and Rutherford (1984) are such examples. However, Elhadi (1984) in his report stated that except for very small streams, it has been shown that complete sectional mixing is not achieved until the pollutant has travelled long distances downstream from the point of release.

The Two-dimensional mixing models developed to-date can be classified according to whether pollutant inputs are steady or unsteady. For example, McCorquodale et al.(1983) developed a mixing model for straight channels and models of Lau and Krishnappan (1981), Somlyody(1982) and Gowda(1984) utilized the stream-tube concept to represent non-uniform, meandering shapes of Rivers. Unsteady-state mixing models include those developed by Verboom (1974), Holly (1975) and Onishi(1981) which deal with straight channels. In addition Holly and Cunge (1975) and Luk et al (1990) developed an unsteady-state stream-tube dispersion model. Also, Harden and Shen (1979) developed a transient mixing model based on a combined implicit, explicit finite difference scheme.

1.3 Objective

This study describes a method of modeling the two-dimensional mixing of pollutants in natural channels, with the use of a simple verification using analytical solutions and a reputed numerical method. The following are the objectives of this study.

1. A 1-D flow simulation model for steady state GVF in an open channel is developed and numerically solved using the Fourth order Runge-Kutta method.

2. A modified form of the MABOCOST model is solved for 1-D flow conditions, with identical lengths of stream tubes at a given cross section, while considering 2-D transverse mixing effects through the transverse mixing coefficient.

3. The pollutant transport is simulated for a straight channel length injected pollutant slugs for conservative and decaying pollutants.

4. The simulated pollutant concentrations for the idealized straight channel configuration is compared with reported experimental and numerical results for 2-D flow in a mildly curved channel with similar cross sections as assumed in this study.

5. The simultion results are also validated using the mass balance criterion for the pollutants.

Chapter 2

Methodology

2.1 Introduction

The flow simulation model considers one-dimensional Gradually Varied Flow and irregular cross sections of the channel. The equation of GVF is non-linear in nature. The Standard Fourth Order Runge-Kutta Method (SRK) is used for the solution of the flow equations for steady state conditions and immobile boundary.

The pollutant transport equation is solved using a modified version of the Mixing Analysis Based On the Concept Of Stream Tubes (MABOCOST) using the time-fractional step method (Luk et al,1990). The governing equations for flow and pollutant transport along with the method of solution used are presented in this chapter.

2.2 Governing Equations for Open Channel Flow

The basic differential equation of GVF is derived from the concept of total energy in open channels. Since the water surface, in general, varies in the longitudinal (x) direction, the depth of flow and total energy are functions of x. The two basic assumptions in the derivation of Gradually Varied Flow equation are:

1. The pressure distribution at any section is assumed to be hydrostatic.

2. At any depth the resistance to flow is assumed to be given by corresponding uniform-flow equation. If Manning's formula is used, the slope term to be used is energy slope but not the bed slope.

The differential equation of GVF also known as the dynamic equation of GVF (Subramanya,1989) is as follows:

$$\frac{dy}{dx} = \frac{S_0 - S_f}{1 - \frac{\alpha Q^2 T}{gA^3}} \tag{2.1}$$

where,

y = depth of flow with respect to a datum

x = longitudinal coordinate

S_0 = the bottom slope of the channel

S_f = the energy slope of the channel flow

α = the kinetic-energy correction factor

Q = the discharge in the channel

T = the top width of flow cross section

g = accelaration due to gravity

A = cross sectional area of discharge

The energy slope is defined as :

$$S_f = \frac{n^2 Q^2}{A^2 R^{4/3}} \tag{2.2}$$

2.3 Governing Equations for Pollutant Transport in Open Channels

In the pollutant transport model the convection can be defined as the transfer of a pollutant from one element in a stream tube to the corresponding element downstream without any change in the total mass. The process of distribution of the pollutant to the adjacent elements without any change in the total mass of the pollutant concentration is known as dispersion. The decay causes reduction in the

total mass of the concentration in each element. In the transport model the pollutant dispersion is governed by the principle of conservation of mass. The continuity equation for neutrally buoyant substance can be written using natural coordinate system (Yotsukura and Sayre, 1976) as :

$$\frac{\partial C}{\partial t} + \frac{u}{m_x}\frac{\partial C}{\partial x} = \frac{\partial}{\partial n}\left(\frac{h^2 u^2 E_z}{Q^2}\frac{\partial C}{\partial n} \right) + \alpha C + \beta \qquad (2.3)$$

This equation the case where the pollutant undergoes a first order chemical reaction, and where either a source or a sink is present owing to localized chemical or biological reactions.

where,

C = depth-averaged pollutant concentration

u = depth-averaged longitudinal velocity

h = local flow depth

E_z = turbulent lateral transverse mixing coefficient

Q = flow rate

α = rate of chemical reactiion

β = magnitude of the source or sink

x = longitudinal coordinate

q = cumulative discharge

n = The non dimensional cumulative discharge

m_x and m_z are the metric coefficients to account for the length variation between coordinate surfaces (for curved channels m_x and m_z are greater than 1.0 , for straight channels $m_x = m_z$=1.0).

The stream tube coordinate system and the schamatic diagram showing stream tubes divided into varible length elements are shown in Fig 2.1 and Fig 2.2 respectively (Luk et al,1990). The nondimensional cumulative discharge 'n' is the fraction of total flow between the bank and the lateral distance z ,that is,

$$n = \frac{q}{Q} = \frac{1}{Q}\int_0^z (m_z h u)dz \qquad (2.4)$$

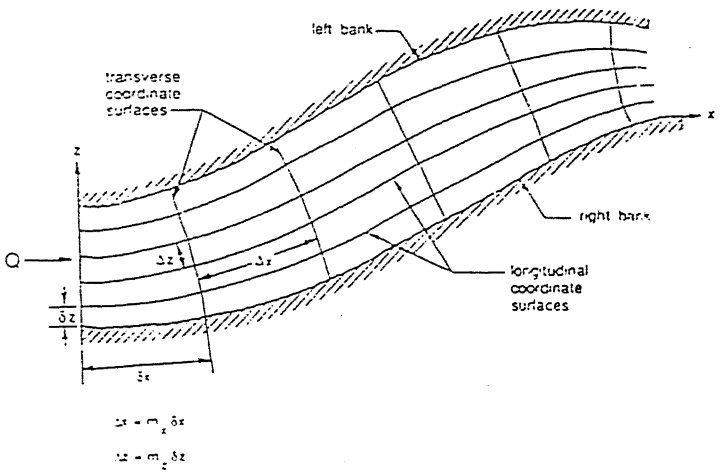


Fig 2.1 Schematic Diagram of the Stream Tubes

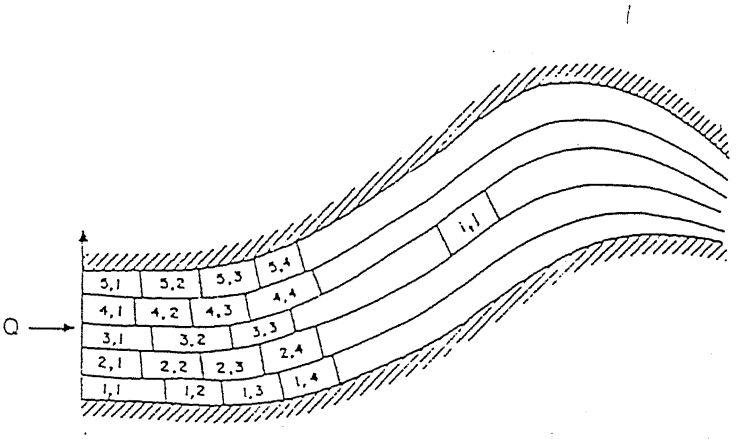


Fig 2.2 Division of stream tubes into variable length elements

The performance of numerical schemes depends on the courant number. In the numerical grid formulated for the finite difference solution of the 2-D mass balance equation the Courant number, L, is defined as :

$$L = \frac{u\Delta t}{\Delta x} \tag{2.5}$$

where,

Δt = time step length and

Δx = longitudinal grid size

Djordjevic and Radojkovic (1986) independently concluded that one of the simplest numerical algorithms that ensures stability and accuracy is the first order, asymmetrical, explicit scheme, with the courant number set to unity throughout the entire grid.

The MABOCOST method is based on the concept of stream tubes. Beltaos (1978) suggested that each stream tube must be divided into the elements with the length of each individual element equal to the product of the local velocity and time interval to satisfy the condition of the Courant number set to unity. The length of each idividual element in the stream tube is defined as :

$$\Delta x = u\Delta t \tag{2.6}$$

In the Eqn.2.3, the longitudinal mixing coefficient is assumed to be negligible as in natural channels the transverse mixing coefficient is few orders of magnitude higher than the longitudinal mixing coefficient.

2.4 Solution Methodology

The solution procedures adopted in this study for solving the flow and pollutant transport equations are discussed in this section. The following assumptions are made for solving the flow equations :

1. The flow in the stream is steady state.

2. The flow is one dimensional.

3. The velocity is constant across a section at any given location.

2.4.1 Methodology for Solution of Flow Model

The 1-D numerical model for open channel flow involves solving the flow equation (Eqn.2.1) using the fourth order Runge-Kutta method.

The fourth order Runge-Kutta method for solving the non-linear differential equation of GVF in open channels is as follows.

$$y_{i+1} = y_i + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) \tag{2.7}$$

where,

$$F(y) = \frac{dy}{dx} \tag{2.8}$$

$$K_1 = \Delta x F(y_i) \tag{2.9}$$

$$K_2 = \Delta x F\left(y_i + \frac{K_1}{2} \right) \tag{2.10}$$

$$K_3 = \Delta x F\left(y_i + \frac{K_2}{2} \right) \tag{2.11}$$

$$K_4 = \Delta x F(y_i + K_3) \tag{2.12}$$

and

y_i = The depth of flow at i^{th} cross section

Δx = The longitudinal step size

Natural channels are, in general, irregular in cross section. In irregulr cross sectional channels the area and top width are functions of the depth of flow. For each depth of flow the area and top width can be obtained graphically or be computed. A table is prepared constituting the area, top width and the corresponding depth for input to the computer. This procedure has been followed at each known cross section for this study.

The channel is divided into N parts of known length interval Δx. Initially, the area of flow and top width are interpolated from the input table corresponding to

given depth of flow. The value of K_1 is evaluated using Eqn. 2.8 for the known depth of flow. Knowing K_1, K_2,K_3 and K_4 are computed using Eqns. 2.10 to 2.12 . Using these computed values of K_1,K_2,K_3 and K_4 and y_i the depth y_{i+1} at the next cross section is obtained. This process is continued for subsequent cross sections. The top width and cross sectional area of flow computing to a given depth y_i is again obtained by interpolation from the table of A and T versus y. The average velocity of flow is determined by using the cross sectional area of flow and discharge values at each cross section.

2.4.2 Methodology for Solution of Pollutant Transport Model

The two-dimensional numerical model for transient pollutant transport involves solving the three computational modules representing advection, dispersion and decay in sequence.

Verboom(1975) showed that the two dimensional mass balance equation (Eqn. 2.3) can be solved by using time fractional-step method. The basic priniciple of this method is the simplification of the solution of a multidimensional mass balance equation by splitting it into many smaller and simpler steps. Stability and consistency of the entire solution can be assured provided the numerical scheme chosen for each indiviual step is stable and consistent.

Some assumptions are made in this transport simulation model. They are :

1. The length of each individual element in each stream tubes is the product of local velocity and time step (maintaining the Courant number as 1.0)

2. The velocity u at any particular cross section as obtained from the solution of the 1-D flow model is uniform across the width. However, for pollutant transport purpose the transverse mixing coefficient E_z is assumed to be non zero to account for actual transverse velocity variation and transverse dispersion.

3. The numerical dispersion and diffusion is avoided with the construction of the grid in a way that the length of each element equal to the distance that pollutant travels in one time step, by advection.

4. The length of the elements in all stream tubes at any particular cross section are equal due to 1-D flow simulation.

A steady reach is divided into a number of stream tubes. Each stream tube is divided into variable length elements at different cross sections. Thus, a numerical grid is formulated with number of stream tubes and elements. The convective portion of the mass balance equation is first solved. The solution is obtained simply by advecting the pollutant forward to the next element, that is

$$C(i,j,t+\Delta t) = C(i,j-1,t) \tag{2.13}$$

where,

i = i^{th} stream tube and

j = j^{th} element in the stream tube.

Following this step, the newly convected element concentrations are dispersed laterally to each of the adjacent elements. This is represented by the following finite difference representation:

$$\begin{aligned} C(i,j,t+\Delta t) &= C(i,j,t) + \frac{\Delta t}{\theta}\sum_{p=1}^{m}\frac{(l\Delta x_l\overline{h\Delta zD\Delta C})_p}{\Delta n_l^2} \\ &+ \frac{(l\Delta x_l)_p|(h\Delta zD)_p - h\Delta zD|\Delta C_p}{\Delta n_l^2} + \sum_{p=1}^{k}\frac{(r\Delta x_r\overline{h\Delta zD\Delta C})_p}{\Delta n_r^2} \\ &+ \frac{(r\Delta x_r)_p|(h\Delta zD)_p - h\Delta zD|\Delta C_p}{\Delta n_r^2} \end{aligned} \tag{2.14}$$

Where,

D = the dispersion factor given by,

$$D = \frac{h^2u^2E_z}{Q^2} \tag{2.15}$$

θ = the volume of an element

Δx = the element length

Δz = the element width

ΔC = the concentration excess and

Δn = the fraction of the cummulative discharge between the centers of two elements

E_z = The transverse mixing coefficient

l,r are the fractions of overlapping area between an element and its adjacent element on the left and right sides, respectively. The subscript p represents the quantities for the p^{th} adjacent elements. the subscripts l and r represent the quantity for the left and right adjacent elements respectively. Overbars represent quantities averaged between an element and its adjacent elements.

Next , the concentrations thus obtained are changed according to a first order chemical reaction or decay.

$$C(i,j,t+\Delta t) = C(i,j,t).exp(\alpha \Delta t) \tag{2.16}$$

Finally the source- sink terms for the current time step can be added to each individual element. These processes are repeated for all time steps to obtain the concentrations for all elements at every time step.

The depth of flow and velocity for each element in a stream tube is calculated by linear interpolation of its depth and velocity obtained by using the SRK method at two sections between which the element is situated. Using these depth and velocities for each idividual element as the input for a given value of transverse mixing coefficient and a time step the dispersive part of the transport model is solved.

The pollutant released in the elements at a given location is convected to the next element in a time step. Following this step, the newly convected element concentrations are dispersed laterally to each of the adjacent elements. Then the growth or the decay takes place. And all these three processes are simultaneous in nature. In each individual element it can be observed that the pollutant concentrations advected to that element go on dispersing and decaying exponentially in each time step. The computer code developed in this study for simulating the transport process is given in Appendix A.

Chapter 3

Solution Results and Discussion

3.1 Introduction

This chapter is devoted to the discussion of the solution results. The flow simulation model assuming steady state GVF in an open channel and the pollutant transport simulation model was applied to an open channel with immobile bed. The cross section of the channel and other details are obtained from the data related to an experimental channel as reported in Luk et al.(1990). The motivation for the same is that experimental observation of actual pollutant movement in a similar channel, however, considering $2-D$ flow in a slightly curved channel has been reported earlier (Luk et al.,1990). Although the simulation results reported here are for a straight channel and considering only $1-D$ channel flow and $2-D$ pollutant transport, those experimental observations provide a basis for comparision of the simulation results.

3.2 Data Used for Simulation

An artificial straight channel with irregular cross section is considered for both flow and transport model simulation. The cross sections are similar to those presented in Luk et al.(1990) for a mildly curved channel. The cross section at upstream end ($X = 0m$) is assumed identical to that at $X = 4m$, from the upstream end for the

simulation purpose, in this study.

In order to relate depth of flow with top width and the flow cross section area, depths of the channel upto $6.25cm$ at $X = 0m$ and$X = 4m$; 8.75 cm at $X = 8m$; and $9.75cm$ at $X = 12m$, respectively were considered. The irregular cross sections of the stream channel, that is, $X = 0m$; $X = 4m$; $X = 8m$; $X = 12m$ are shown in $Fig3.1$. The experimental channel as reported in Luk et al.(1990) followed a sine curve with a wavelength of $1.9m$ and amplitude of $0.29m$. The channel was $0.3m$ wide, with irregular bottom features. The channel was located in a $3mX20m$ sand basin with a sloping bed and sheet metal side walls. A conatant flow was discharged into the channel to scour the bed features naturally. Sand was fed in at the upstream end at a rate as close as possible to the erosion rate. After equilibrium was established, the water was drained and the features were preserved by spraying a dilute resin solution on the bed. It was hardened with a dilute solution of formic acid resulting in a hard bottom. For the simulation in this study, the same cross sections were considered, with a straight longitudinal profile. The slope and discharge remain the same.

In the flow simulation model the Manning's coefficient of roughness, n is assumed to be 0.010 for an artificial channel. As the cross sections are given at an interval of $4m$ the same step size of $4m$ in the length direction is assumed. The paramaters used in the flow simulation model are presented in $Table3.1$.

Description	Parameter
Discharge in the channel, Q	0.00396 m^3/s
Accelaration due to gravity, g	9.81 m/s^2
Channel bottom slope, S_0	0.0035
Kinetic-energy correction factor, α	1.0

Table 3.1 : Flow Parameter Values

In the transport simulation model the stream is divided into seven stream tubes. Each stream tube is $0.0428m$ wide with a number of varying length elements.

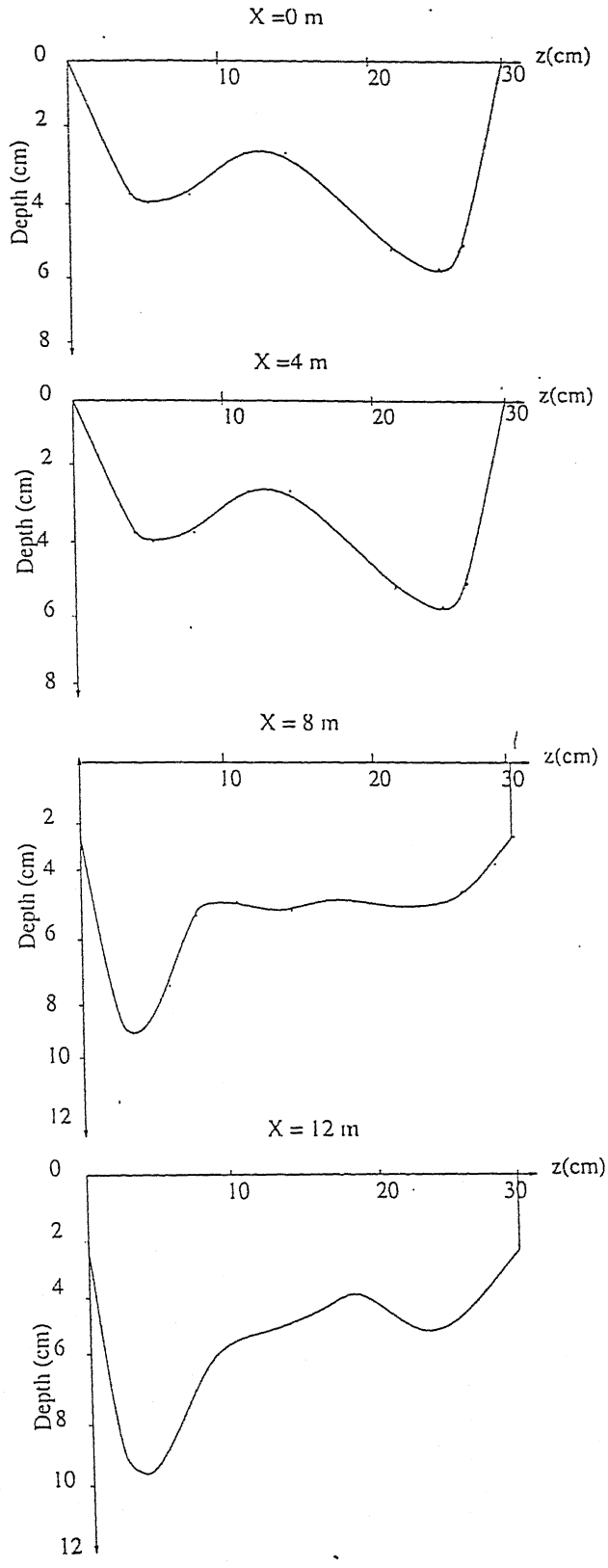


Fig 3.1 Channel Sections

The length of each element is the product of local velocity and the time step. The flow simulation model is one dimensional resulting in no velocity variation along a given cross section. Therefore, the length of stream tubes remain same at a given cross section. The time step is assumed to be $1 second$ in the transport model. The input data for this model is presented in the $Table 3.2$.

Description	Parameter
Width of the stream channel	0.3 m
Flow rate, Q	0.00396 m^3/s
Averaged flow depth, h	0.04 m
Average flow velocity, u	0.35 m/s
Mean bed slope, S_0	0.0035
Number of stream tubes	7
Concentration in 3^{rd}st.tube	495.51 mg/L
Concentration in 4^{th}st.tube	1123.7 mg/L
Concentration in 5^{th}st.tube	2317.33 mg/L
Time step, Δt	1 sec.
Transverse mixing coefficient, E_z	0.00021 m^2/s
Rate of chemical reaction, α	0.0 s^{-1}

Table 3.2 : Pollutant Transport Parameter Values

The transverse mixing coefficient, E_z, used in this model is assumed to be non zero since the transport model is $2-D$ and there is transverse movement of the concentrations bacause of dispersion even though the average velocity across any cross section is uniform, as the flow simulation model is $one-dimensional$. The mixing coefficient can however, account for transverse velocity variation, unmodelled in the $1-D$ simulation model. The flow simulation is assumed to be steady state, while the transport simulation model is transient. The E_z value is taken identical to the value used for the $2-D$ flow in the experimental channel, so that the mixing effects are atleast accounted for in the transport model.

A slug injection is an insertion of certain concentration instantaneously. A continous injection can be considered as an aggregate of infinite number of slug injections at a very small time interval. In this study single or multiple slug injections are considered for simulation purpose. It is assumed that the slug is injected at time $t = 1second$ in three adjacent stream tubes on either side of the central stream tube, that is,3^{rd}, 4^{th} and 5^{th} stream tubes to simulate better mixing affects. This is because in the modelled $one - dimensional$ flow, complete mixing cannot take place until the pollutant has travelled long distances downstream from the point of release.

3.3 Simulation Results

The computations are carried out with an initial maximum depth of $2.65cm$ in the upstream cross section ($X = 0m$) measured from the bottom most point of the stream channel bed. The average velocity is higher at this cross section since the area of flow is lower for steady flow conditions to be maintained. In the experimental results (Luk et al.,1990), the depth profile and channel cross section at $X = 0m$ is not reported. Therefore, cross sections are assumed to be identical at $X = 0m$ and $X = 4m$, in this study. The depth of $2.65cm$ at $X = 0m$ is obtained by iterative trial and error solution of the flow simulation model so as to achieve depth profiles at $X = 8m$ and $X = 12m$ as obtained for the experimental channel.

Since the model is $one - dimensional$ a uniform average velocity is simulated at any particular cross section. The depth profiles are well matched with the experimental data at the downstream sections. The maximum depth of flow at $X = 8m$ is observed as $6.788cm$. This differs from the experimental value by less than $1percent$. A depth of flow at $X = 12m$ is obtained as $7.760cm$. This depth of flow differs by a still lesser value, that is $0.5percent$. These results clearly indicate that the simulation model results are well matched on the downstream sections. In this model a decreasing average velocity can be observed along the direction of flow due to the increasing cross sectional area along the direction of flow. These results are intutively

expected in natural channels also.

In the pollutant transport model $0.1L$ of a tracer solution with a concentration of $58000mg/L$ is injected in three adjacent stream tubes, that is, 3^{rd}, 4^{th} and 5^{th} stream tubes for better simulation. The results show that at $X = 4m$ from the upstream side, complete sectional mixing is not achieved and hence the peaks in the concentration profiles are higher in certain stream tubes in which the slug is inserted at $X = 0m$. In the remaining stream tubes the peaks are comparitively lower. Further downstream, peaks are less concentrated in those stream stream tubes in which the pollutant was released upstream. Also, the pollutant spread in the transverse direction due to dispersion effects. The concentration profiles at a section $X = 12m$ show further dispersion of the pollutant. The time-concentration profiles obtained for this simulation model as well as for both the MABOCOST and experimental models are shown in $Fig3.2$. A usual comparison of the concentration profiles (break through curves) show that in the combined use of $1-D$ flow and $2-D$ transport model, assuming a straight longitudinal profile, the peaks are higher compared to MABOCOST and experimental results. However, again due to reduced mixing on dispersion effects, the time base of the break through curves are shorter in these simulations. It is also observed that the peaks are achieved faster in the central stream tubes. In the of-centre stream tubes peaks are lower than the MABOCOST and experimental results, also due to the lack of transverse velocity in the flow modelled.

The computational results for estimating total mass of the pollutant at a cross section $X = 4m$ is presented in the $Table3.3$. The pollutant concentration in an element at any section is the product of discharge and area under the time-concentration curve for that element. The discharge per second passing through an element is equal to its volume for steady flow conditions (as $\Delta t = 1sec.$). The

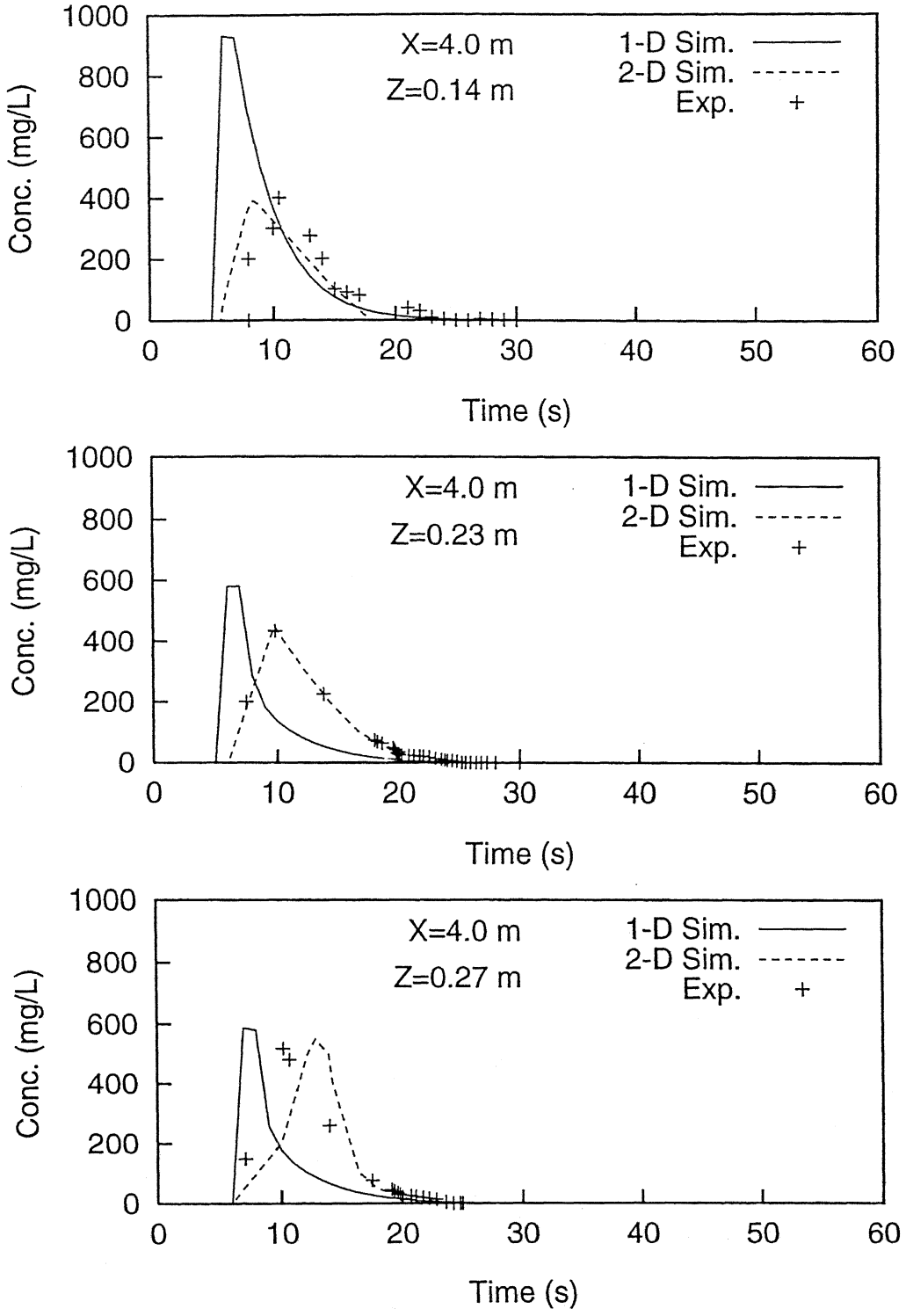


Fig 3.2 Comparison of Simulation Results with Experimental and original MABOCOST Results

(cont

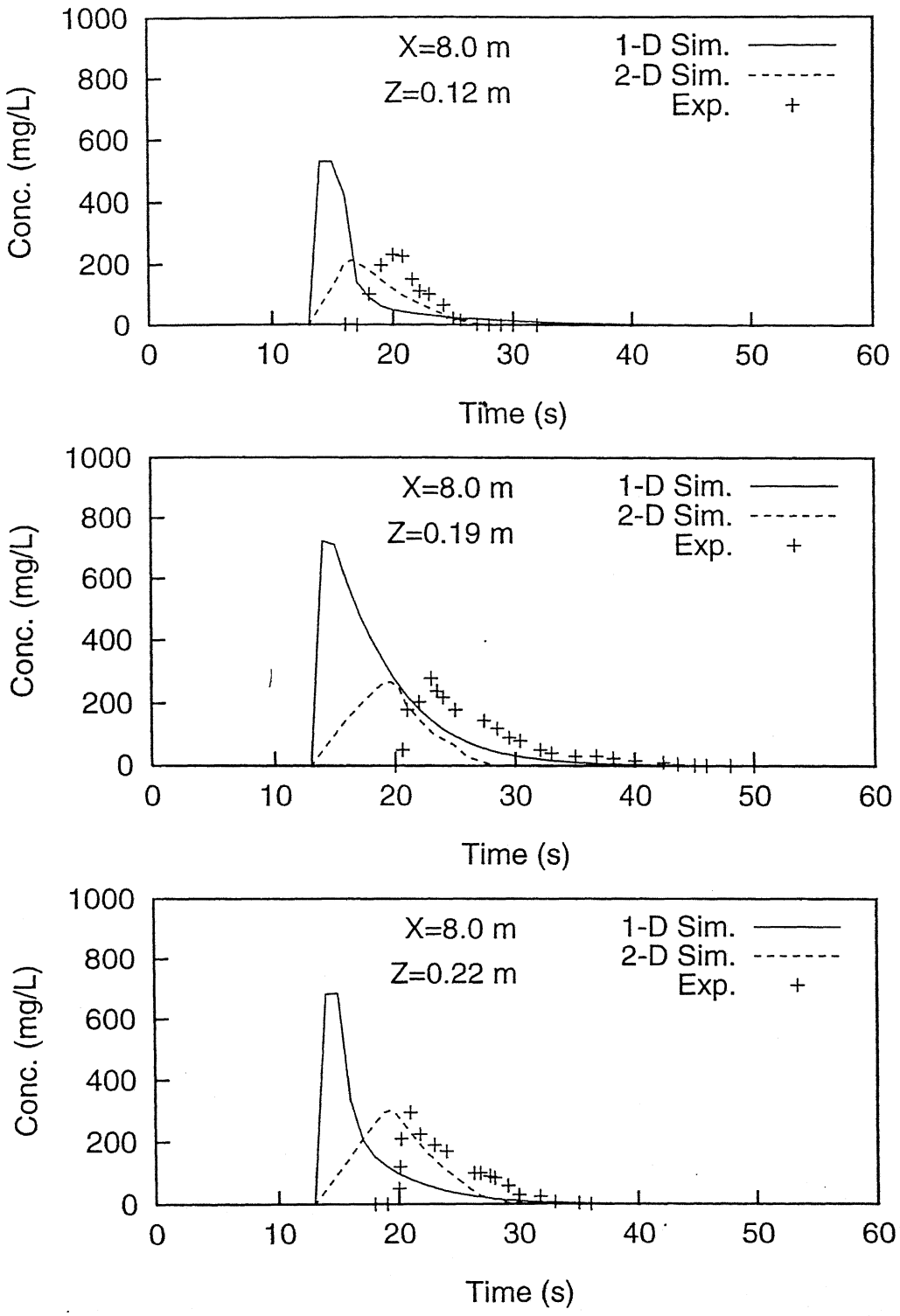


Fig 3.2 Comparison of Simulation Results with Experimental and original MABOCOST Results

(contd

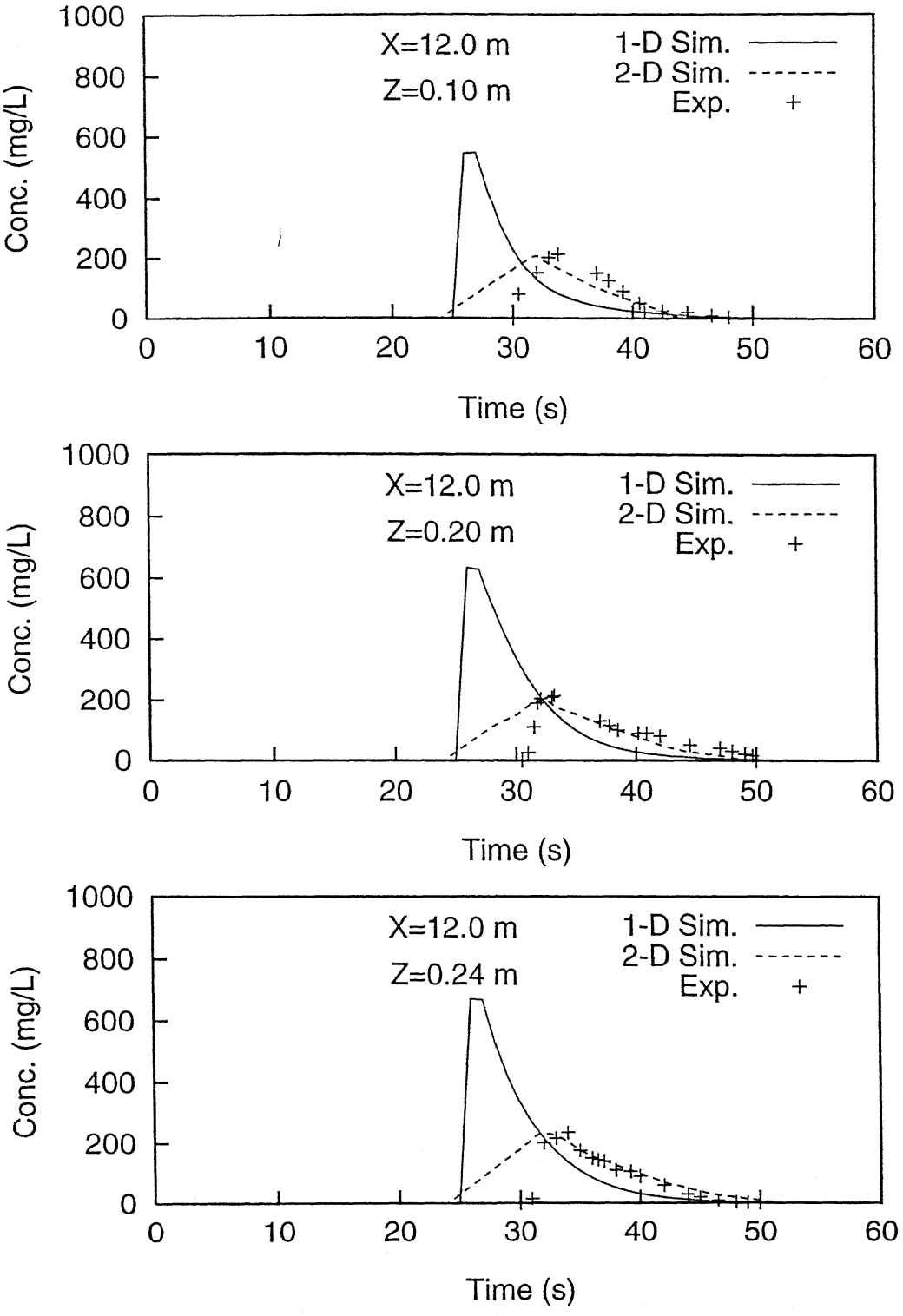


Fig 3.2 Comparison of Simulation Results with Experimental and original MABOCOSTResult

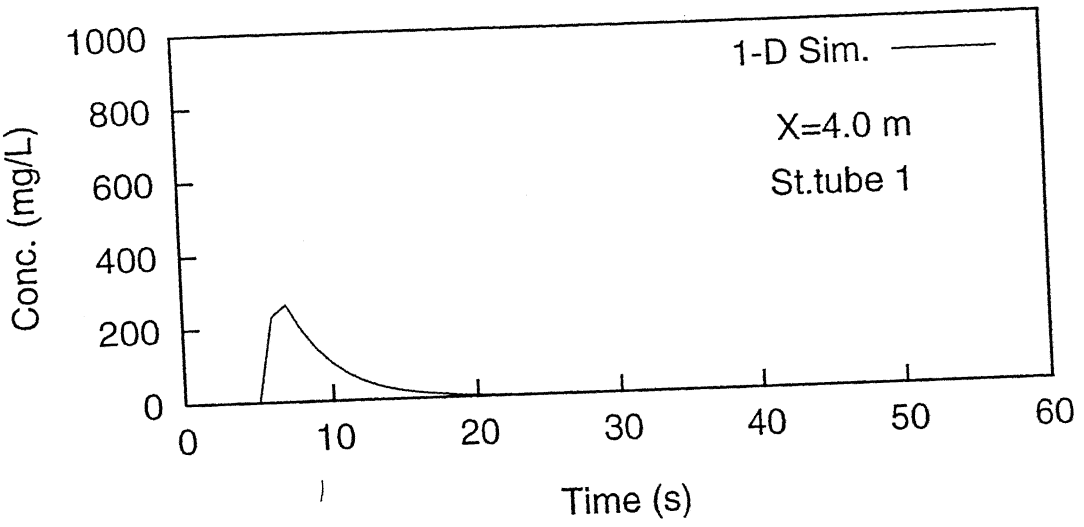
St.tube number (1)	Area under Time-Conc. curve (mg-sec./L) (2)	Discharge (L/sec.) (3)	Mass (mg) (2 X 3) (4)
1	769.125	0.311	239.19
2	1136.85	0.529	601.39
3	1727.56	0.407	703.11
4	2708.36	0.504	1365.01
5	2653.91	0.712	1889.58
6	1375.47	0.863	1187.03
7	1367.90	0.458	626.44
		Total mass	6611.80

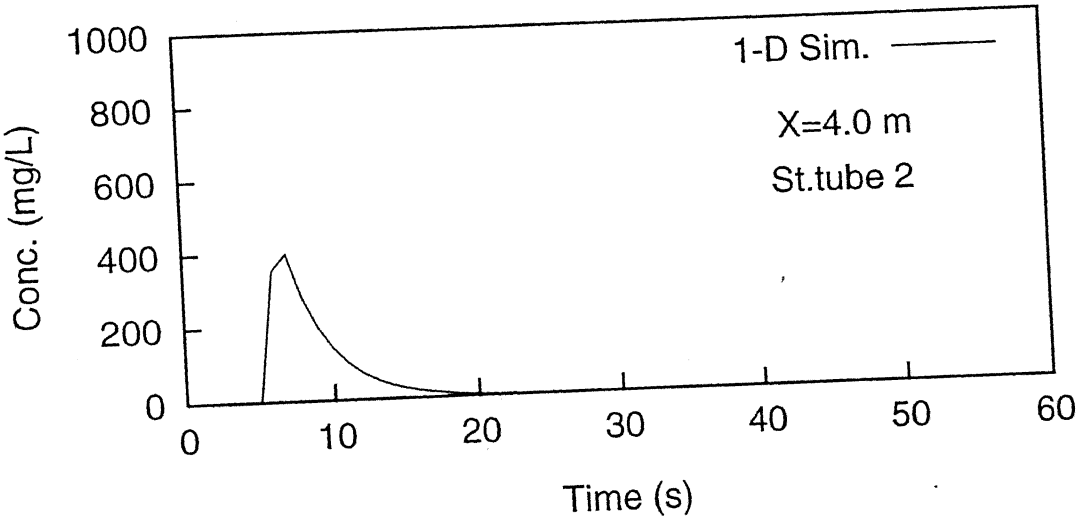
Table 3.3 : Mass Balance Calculations

results show that the total mass of simulated pollutant concentration at this section differs by approximately 13% when compared with the input mass at $X = 0m$. Also, this difference at $X = 8m$ is observed as 11.87%. This mass balance error can be considered to be within the acceptable range for numerical simulation.The concentration profiles for all the stream tubes at $X = 4m$ are given in Fig 3.3

Another illustrative example with varying decay factors 0.1 and 0.05 show decreasing concentrations downstream of the channel when compared with those obtained without considering any decay. These profiles are shown in *Fig*3.4. A change in the growth or decay factor affects the advected values to the neighbouring elements in the flow direction. For conservative pollutants this factor is kept *zero* since no growth or decay takes place.

The transport model is also tested for a case of two slugs injected at 10 seconds interval with same concentration and input as reported earlier. These results show two peaks in each profile with the second peak slightly higher than the first one because of a small residual concentrations left over at various sections at the time of second slug injection. The concentration profiles are shown in the *Fig*3.5.





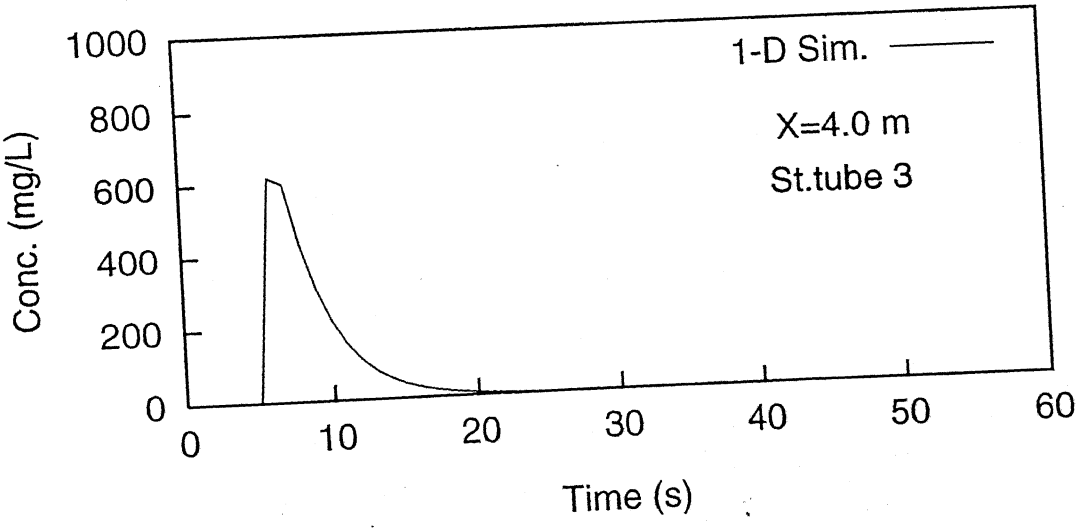


Fig 3.3 Concentrarion Profiles for all Stream Tubes at $X = 4m$ (contd.)

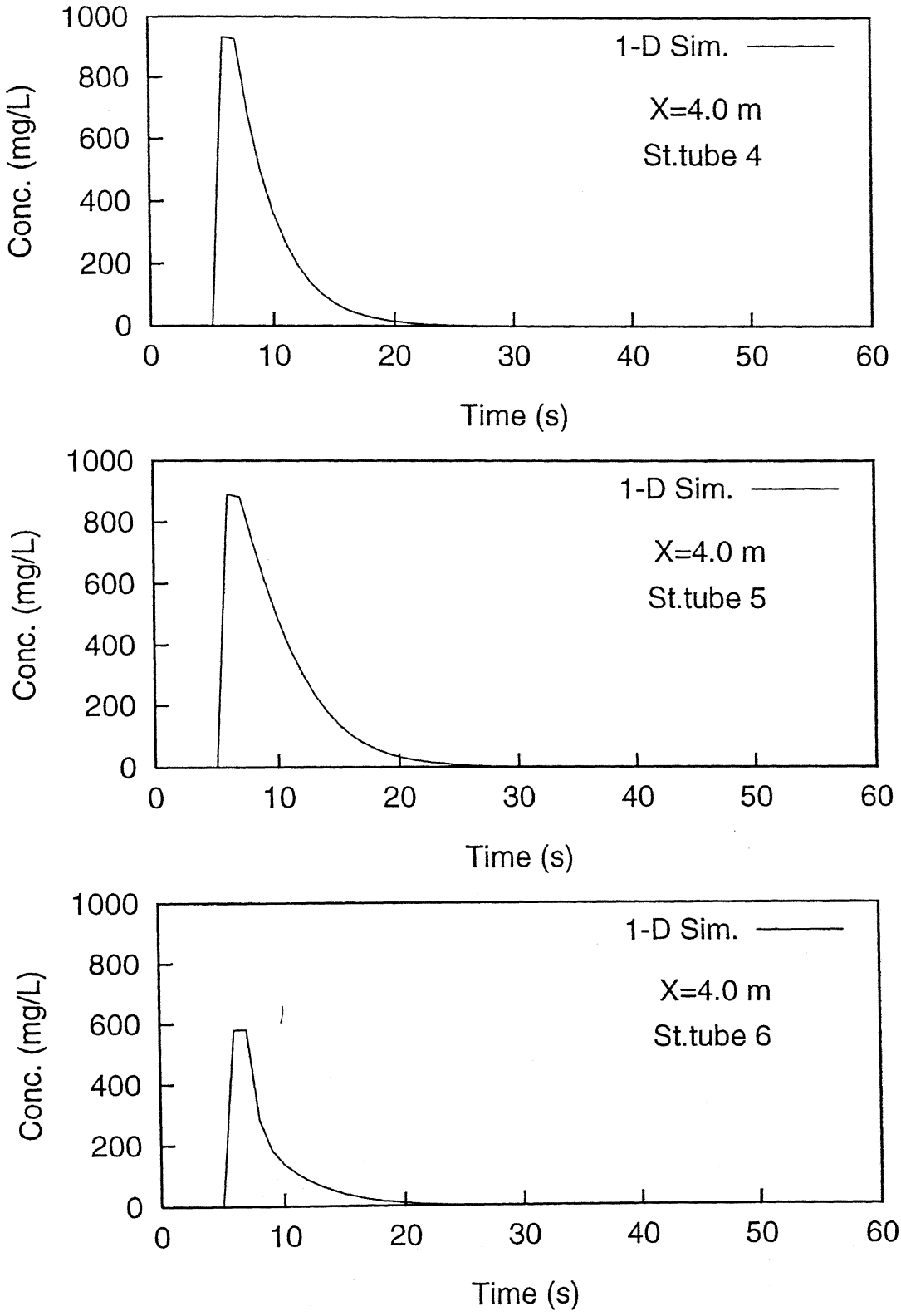


Fig 3.3 Concentrarion Profiles for all Stream Tubes at X = 4m

(contd.)

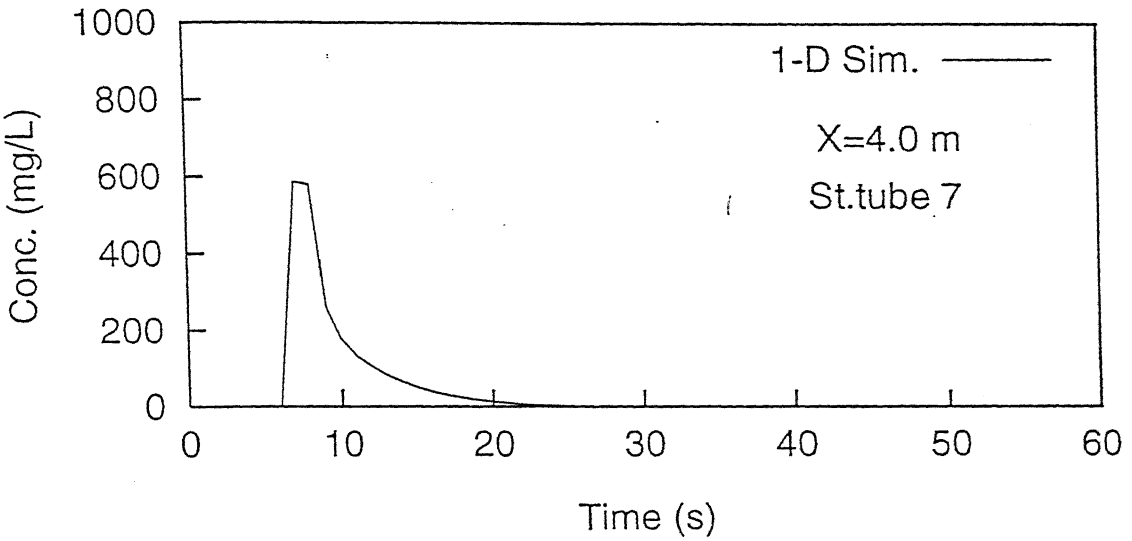


Fig 3.3 Concentration Profiles for all Stream Tubes at X = 4m

It is apparent from the previous discussion that $1-D$ flow and $2-D$ transport simulation gives comparable results with respect to the actual experimental data and can provide acceptable intial results before a more sophisticated $2-D$ flow modelling is attempted. This is a viable method for pollutant simulation in wide open channels especially during dry seasons, when flow is nearly steady GVF, but water quality is a critical factor.

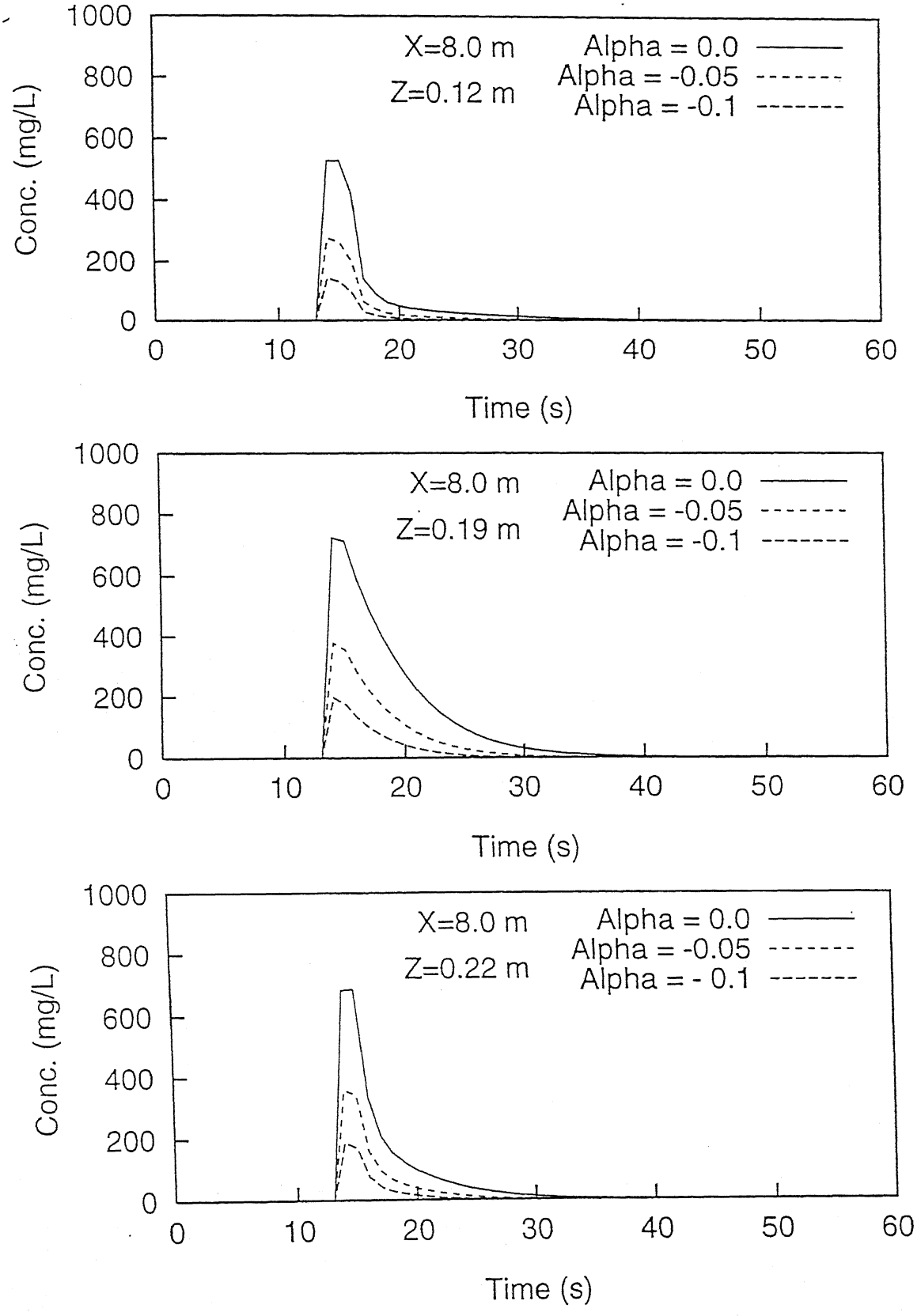


Fig 3.4 Comparision of Simulation Concentrations at X = 8m for different α

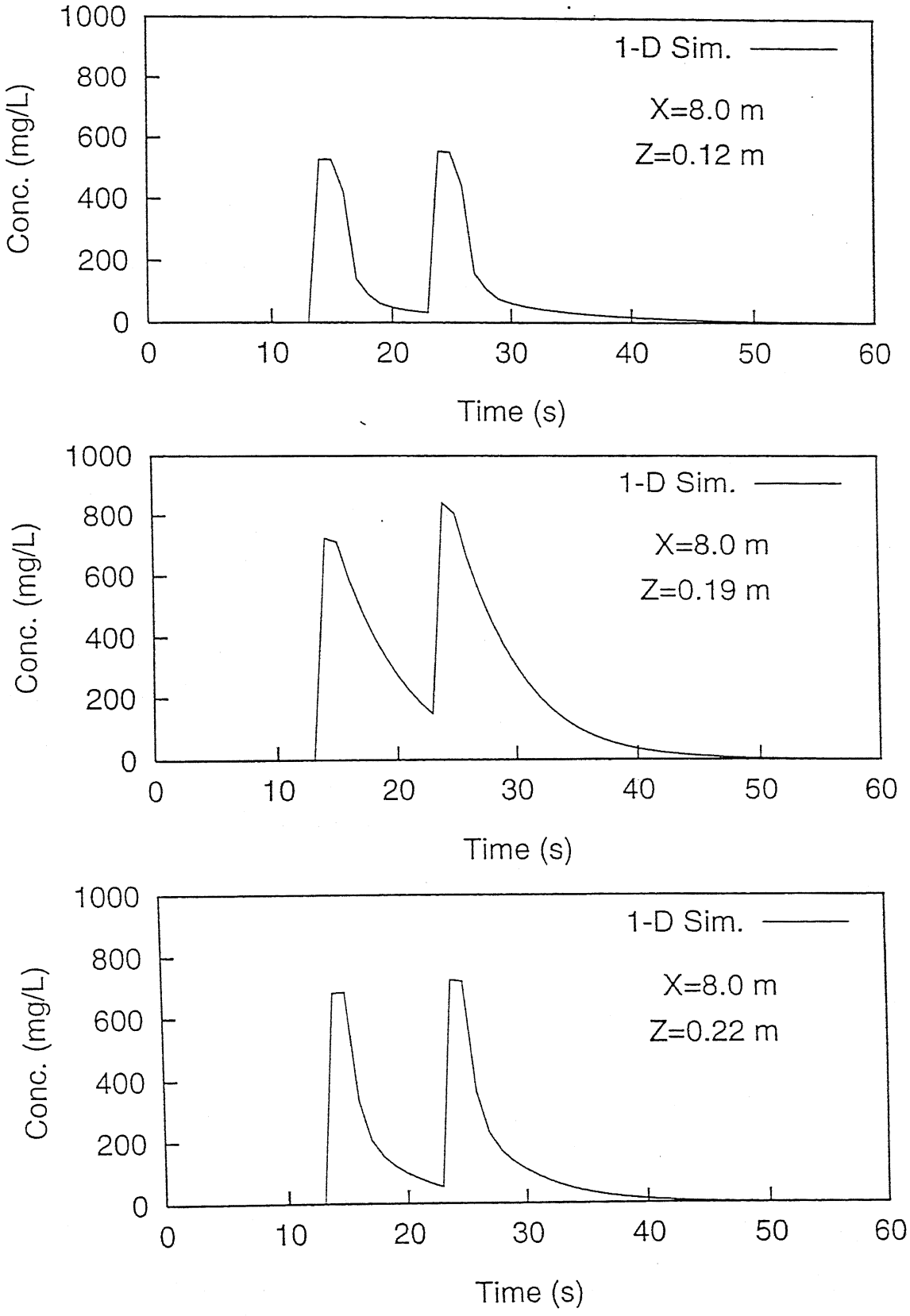


Fig 3.5 Concentration Profiles for Multiple Slug Injections

Chapter 4

Summary and Conclusions

4.1 Summary

In this study (i) A numerical model is developed for simulating $1-D$ flow under steady state conditions for channels with irregular cross sections (ii) A simulation model is solved for simulating the $2-D$ transport of a pollutant in the channel. This model is applicable for both $1-D$ and $2-D$ flow systems using the stream tube concept.

The flow simulation model is formulated using the fourth order Runge Kutta method. The flow model is solved for an open channel with specified irregular cross sections assuming immobile bed conditions. The transport simulation model utilizes the flow simulation solutions to simulate pollutant transport in the channel, assuming advective and dispersive transport processes.

The numerical solution is based on the modification of solution procedure suggested earlier for Mixing Anlysis Based on the Concept of Stream Tubes (MABOCOST) in a $2-D$ environment. The transport model simulates the spatial and temporal distribution of pollutant concentration for given pollution sources. The simulated results are compared with reported experimental results for a similar $2-D$ system as well as reported $2-D$ simulation results using MABOCOST. These comparisons and mass balance analysis show that the combined $1-D$ flow and $2-D$ pollutant transport simulation results may be used as approximate solu-

tions for the $2-D$ system for preliminary assessment. Both conservative pollutants and pollutants undergoing decay process are considered.

4.2 Conclusions

This study shows the potential applicability of a $1-D$ open channel flow simulation model and a $2-D$ pollutant transport simulation model for obtaining preliminary solution for an open channel system with $2-D$ flow. The feasibility of solving these two models in conjunction for conservative and non conservative pollutants are demonstrated using illustrative examples. Mass balance considerations validate the solution results for the illustrative problem.

The $1-D$ flow and $2-D$ transport model gives comparable results $vis-a-vis$ experimentally observed data for a $2-D$ flow system. This conclusions may not be valid when the transverse velocities are significant.

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APPENDIX A

```
*       Program for 2-D Pollutant Transport Simulation Model

*       ------------------------------------------------------

*       DECLARATION

        double precision tc(50,50,100),fc(50,50,50)
        double precision wc(20),xc(20),yc(20),zc(20)
        double precision wh(20),xh(20),yh(20),zh(20)
        double precision wu(20),xu(20),yu(20),zu(20)
        double precision zl(20,100),zr(20,100)
        double precision h(20,100),u(20,100)
        double precision d(20,100),dx(20,100)
        double precision dnl(20,100),dnr(20,100)
        double precision theta(20,100)
        double precision dz,z,l,r,ez,q,x
        double precision alpha,beta
        double precision slef,srt
        integer time,dt,imax,jmax
        integer is,je,lt
*       ------------------------------------------------------

        common/first/h,u,d,dx
        common/second/dz,z,l,r,q
        common/third/time,dt,imax,jmax
        common/fourth/zl,zr
        common/fifth/dnl,dnr
*       ------------------------------------------------------
```

```
      open(unit=9,file="zero")
      open(unit=10,file="four")
      open(unit=11,file="eight")
      open(unit=12,file="twelve")
      open(unit=13,file="input")
      open(unit=14,file="conc")
      open(unit=15,file="output")

*     Enter the following parameters
      read (13,*)imax,time,dt,ez,q,dz,z,alpha,beta
      do 10 i=1,imax
      read(9,*)wc(i),wh(i),wu(i)
      read(10,*)xc(i),xh(i),xu(i)
      read(11,*)yc(i),yh(i),yu(i)
      read(12,*)zc(i),zh(i),zu(i)
10    continue
      x=0.0
      ltn=1
21    do 20 ib=1,imax
      if((x.ge.0.0).and.(x.lt.4.0))then
      tc(ib,ltn,1)=wc(ib)+((x-0)/4.0)*(xc(ib)-wc(ib))
      h(ib,ltn)=wh(ib)+((x-0)/4.0)*(xh(ib)-wh(ib))
      u(ib,ltn)=wu(ib)+((x-0)/4.0)*(xu(ib)-wu(ib))
      elseif((x.ge.4.0).and.(x.lt.8.0))then
      tc(ib,ltn,1)=xc(ib)+((x-4)/4.0)*(yc(ib)-xc(ib))
      h(ib,ltn)=xh(ib)+((x-4)/4.0)*(yh(ib)-xh(ib))
      u(ib,ltn)=xu(ib)+((x-4)/4.0)*(yu(ib)-xu(ib))
      elseif((x.ge.8.0).and.(x.le.12.0))then
      tc(ib,ltn,1)=yc(ib)+((x-8)/4.0)*(zc(ib)-yc(ib))
      h(ib,ltn)=yh(ib)+((x-8)/4.0)*(zh(ib)-yh(ib))
```

```
      dx(ib,ltn)=u(ib,ltn)*dt
      d(ib,ltn)=((h(ib,ltn)**2)*(u(ib,ltn)**2)*ez)/(q**2)
      theta(ib,ltn)=dx(ib,ltn)*dz*h(ib,ltn)
      if(x.le.12.0)then
      jmax=ltn
      endif
20    continue
      if(x.gt.12.0)then
      goto 22
      else
      write(*,*)ltn,x
      x=x+dx(1,ltn)
      ltn=ltn+1
      goto 21
      endif
22    write(*,*)'At what location no.of st.tub,elment'
      read(*,*)mst,mel
      read(14,*)(tc(i,j,mt),i=3,5)
      it=1
      num=1
      goto 25
15    do 30 ii=1,imax
      tc(ii,num,it)=tc(ii,num-1,it)
30    continue
25    do 40 is=1,imax
      je=num
      do 35 lt=it,time,dt
      call left(tc,is,je,lt,slef)
      call right(tc,is,je,lt,srt)
      tc(is,je,lt+dt)=tc(is,je,lt)+(dt/theta(is,je))*(srt+slef)
```

```
      tc(is,je,lt+dt)=tc(is,je,lt+dt)*exp(alpha*dt)
35    continue
40    continue
      it=it+dt
      num=num+1
      if(num.gt.jmax)goto 45
      goto 15
45    do 50 kt=1,time,dt
      write(15,100)kt,tc(mst,mel,kt)
100   format(2x,'Time',2x,i5,2x,'Concentration',2x,f8.2)
50    continue
      stop
      end

      subroutine left(tc,is,je,lt,slef)
*     ------------------------------------------------------

*     DECLARATION

      double precision tc(50,50,100),fc(50,50,50)
      double precision zl(20,100),zr(20,100)
      double precision h(20,100),u(20,100)
      double precision d(20,100),dx(20,100)
      double precision delc(20,100)
      double precision dnl(20,100),dnr(20,100)
      double precision dz,z,l,r,q
      double precision slef,srt
      integer time,dt,imax,jmax,p
      integer is,je,lt
*     ------------------------------------------------------
```

```
      common/first/h,u,d,dx
      common/second/dz,z,l,r,q
      common/third/time,dt,imax,jmax
      common/fourth/zl,zr
      common/fifth/dnl,dnr
*     ------------------------------------------------------

      do 200 mi=1,imax
      do 220 mj=1,jmax
      if(mi.le.1)then
      delc(mi,mj)=tc(mi,mj,lt)
      dnl(mi,mj)=h(mi,mj)*u(mi,mj)*dz/q
      else
      gl=0.0
      do 225 isk=1,mi
      gl=gl+h(isk,mj)
225   continue
      gm=0.0
      mik=mi-1
      do 230 isl=1,mik
      gm=gm+h(isl,mj)
230   continue
      dnl(mi,mj)=(gm-gl)*u(mi,mj)*dz/q
      delc(mi,mj)=(tc(mi-1,mj,lt)-tc(mi,mj,lt))
      endif
220   continue
200   continue
      l=1
      m=1
```

```
      do 250 p=1,m
      if(is.le.1)then
      slef=0.0
      else
      avgl=(h(is,je)*d(is,je)+h(is-1,je)*d(is-1,je))/2.0
      prodl=l*dx(is-1,je)*avgl*dz*delc(is,je)
      ft=prodl/(dnl(is,je)**2)
      ftemp=((h(is-1,je)*dz*d(is-1,je))-(h(is,je)*dz*d(is,je)))
      ftemp=abs(ftemp)
      sd=(l*dx(is-1,je)*ftemp*delc(is,je))/(dnl(is,je)**2)
      slef=ft+sd
      endif
250   continue
      return
      end

      subroutine right(tc,is,je,lt,srt)

*     ------------------------------------------------------------

*     DECLARATION

      double precision tc(50,50,100),fc(50,50,50)
      double precision zl(20,100),zr(20,100)
      double precision h(20,100),u(20,100)
      double precision d(20,100),dx(20,100)
      double precision rdc(20,100)
      double precision dnl(20,100),dnr(20,100)
      double precision dz,z,l,r,q
      double precision slef,srt
```

```
      integer time,dt,imax,jmax,p
      integer is,je,lt

*     ------------------------------------------------------------

      common/first/h,u,d,dx
      common/second/dz,z,l,r,q
      common/third/time,dt,imax,jmax
      common/fourth/zl,zr
      common/fifth/dnl,dnr
*     ------------------------------------------------------------

      do 300 il=1,imax
      do 320 jl=1,jmax
      if(il.ge.imax)then
      rdc(il,jl)=tc(il,jl,lt)
      dnr(il,jl)=h(il,jl)*u(il,jl)*dz/q
      else
      rdc(il,jl)=(tc(il+1,jl,lt)-tc(il,jl,lt))
       vb=0.0
       do 325 jsk=1,il
       vb=vb+h(jsk,jl)
325    continue
       vc=0.0
       ilm=il+1
       do 330 jsl=1,ilm
       vc=vc+h(jsl,jl)
330    continue
       dnr(il,jl)=(vc-vb)*u(il,jl)*dz/q
       endif
```

```
 300    continue
        r=1
        k=1
        do 350 p=1,k
        if(is.ge.imax)then
        srt=0.0
        else
        ravg=(h(is,je)*d(is,je)+h(is+1,je)*d(is+1,je))/2.0
        rmult=r*dx(is+1,je)*dz*rdc(is,je)*ravg
        rtd=rmult/(dnr(is,je)**2)
        serve=((h(is+1,je)*dz*d(is+1,je))-(h(is,je)*dz*d(is,je)))
        serve=abs(serve)
        fth=(r*dx(is+1,je)*serve*rdc(is,je))/(dnr(is,je)**2)
        srt=rtd+fth
        endif
 350    continue
        return
        end

        * * *
```

TYPICAL INPUT TABLE :

```
7 100 1 0.00021 0.00396 0.04285 0.0 0.0

495.51
1123.8
2317.33
```